



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Aug 10, 2019 – 10:41 PM EDT

PDB ID : 6H3C
EMDB ID: : EMD-0132
Title : Cryo-EM structure of the BRISC complex bound to SHMT2
Authors : Bunker, R.D.; Rabl, J.; Thoma, N.H.
Deposited on : 2018-07-18
Resolution : 3.90 Å(reported)
Based on PDB ID : 6GVW, 5V7I

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

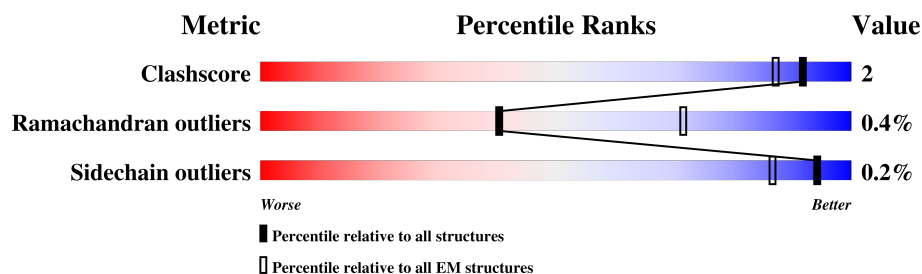
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	434	53% 5% 41%
1	F	434	54% . 41%
2	B	335	72% 5% 23%
2	G	335	72% 5% 23%
3	C	402	84% 10% . 5%
3	H	402	83% 11% . 5%
4	D	352	61% 6% . 33%
4	I	352	62% 5% . 33%
5	E	507	80% 7% 13%

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Mol	Chain	Length	Quality of chain
5	J	507	<div><div></div><div>79%</div><div>7%</div><div>13%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49982 atoms, of which 24860 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BRISC complex subunit Abraxas 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	255	Total	C	H	N	O	S	0	0
			4134	1305	2052	375	395	7		
1	F	255	Total	C	H	N	O	S	0	0
			4134	1305	2052	375	395	7		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q15018
A	-17	HIS	-	expression tag	UNP Q15018
A	-16	HIS	-	expression tag	UNP Q15018
A	-15	HIS	-	expression tag	UNP Q15018
A	-14	HIS	-	expression tag	UNP Q15018
A	-13	HIS	-	expression tag	UNP Q15018
A	-12	HIS	-	expression tag	UNP Q15018
A	-11	VAL	-	expression tag	UNP Q15018
A	-10	ASP	-	expression tag	UNP Q15018
A	-9	GLU	-	expression tag	UNP Q15018
A	-8	ASN	-	expression tag	UNP Q15018
A	-7	LEU	-	expression tag	UNP Q15018
A	-6	TYR	-	expression tag	UNP Q15018
A	-5	PHE	-	expression tag	UNP Q15018
A	-4	GLN	-	expression tag	UNP Q15018
A	-3	GLY	-	expression tag	UNP Q15018
A	-2	GLY	-	expression tag	UNP Q15018
A	-1	GLY	-	expression tag	UNP Q15018
A	0	ARG	-	expression tag	UNP Q15018
F	-18	MET	-	initiating methionine	UNP Q15018
F	-17	HIS	-	expression tag	UNP Q15018
F	-16	HIS	-	expression tag	UNP Q15018
F	-15	HIS	-	expression tag	UNP Q15018
F	-14	HIS	-	expression tag	UNP Q15018
F	-13	HIS	-	expression tag	UNP Q15018
F	-12	HIS	-	expression tag	UNP Q15018

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	VAL	-	expression tag	UNP Q15018
F	-10	ASP	-	expression tag	UNP Q15018
F	-9	GLU	-	expression tag	UNP Q15018
F	-8	ASN	-	expression tag	UNP Q15018
F	-7	LEU	-	expression tag	UNP Q15018
F	-6	TYR	-	expression tag	UNP Q15018
F	-5	PHE	-	expression tag	UNP Q15018
F	-4	GLN	-	expression tag	UNP Q15018
F	-3	GLY	-	expression tag	UNP Q15018
F	-2	GLY	-	expression tag	UNP Q15018
F	-1	GLY	-	expression tag	UNP Q15018
F	0	ARG	-	expression tag	UNP Q15018

- Molecule 2 is a protein called Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	258	Total	C	H	N	O	S	0	0
			4122	1295	2053	366	394	14		
2	G	258	Total	C	H	N	O	S	0	0
			4122	1295	2053	366	394	14		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP P46736
B	-17	HIS	-	expression tag	UNP P46736
B	-16	HIS	-	expression tag	UNP P46736
B	-15	HIS	-	expression tag	UNP P46736
B	-14	HIS	-	expression tag	UNP P46736
B	-13	HIS	-	expression tag	UNP P46736
B	-12	HIS	-	expression tag	UNP P46736
B	-11	VAL	-	expression tag	UNP P46736
B	-10	ASP	-	expression tag	UNP P46736
B	-9	GLU	-	expression tag	UNP P46736
B	-8	ASN	-	expression tag	UNP P46736
B	-7	LEU	-	expression tag	UNP P46736
B	-6	TYR	-	expression tag	UNP P46736
B	-5	PHE	-	expression tag	UNP P46736
B	-4	GLN	-	expression tag	UNP P46736
B	-3	GLY	-	expression tag	UNP P46736
B	-2	GLY	-	expression tag	UNP P46736
B	-1	GLY	-	expression tag	UNP P46736

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ARG	-	expression tag	UNP P46736
G	-18	MET	-	initiating methionine	UNP P46736
G	-17	HIS	-	expression tag	UNP P46736
G	-16	HIS	-	expression tag	UNP P46736
G	-15	HIS	-	expression tag	UNP P46736
G	-14	HIS	-	expression tag	UNP P46736
G	-13	HIS	-	expression tag	UNP P46736
G	-12	HIS	-	expression tag	UNP P46736
G	-11	VAL	-	expression tag	UNP P46736
G	-10	ASP	-	expression tag	UNP P46736
G	-9	GLU	-	expression tag	UNP P46736
G	-8	ASN	-	expression tag	UNP P46736
G	-7	LEU	-	expression tag	UNP P46736
G	-6	TYR	-	expression tag	UNP P46736
G	-5	PHE	-	expression tag	UNP P46736
G	-4	GLN	-	expression tag	UNP P46736
G	-3	GLY	-	expression tag	UNP P46736
G	-2	GLY	-	expression tag	UNP P46736
G	-1	GLY	-	expression tag	UNP P46736
G	0	ARG	-	expression tag	UNP P46736

- Molecule 3 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	383	Total	C	H	N	O	S	0	0
			6077	1993	2999	504	567	14		
3	H	383	Total	C	H	N	O	S	0	0
			6077	1993	2999	504	567	14		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	initiating methionine	UNP Q9NXR7
C	-17	HIS	-	expression tag	UNP Q9NXR7
C	-16	HIS	-	expression tag	UNP Q9NXR7
C	-15	HIS	-	expression tag	UNP Q9NXR7
C	-14	HIS	-	expression tag	UNP Q9NXR7
C	-13	HIS	-	expression tag	UNP Q9NXR7
C	-12	HIS	-	expression tag	UNP Q9NXR7
C	-11	VAL	-	expression tag	UNP Q9NXR7
C	-10	ASP	-	expression tag	UNP Q9NXR7
C	-9	GLU	-	expression tag	UNP Q9NXR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	ASN	-	expression tag	UNP Q9NXR7
C	-7	LEU	-	expression tag	UNP Q9NXR7
C	-6	TYR	-	expression tag	UNP Q9NXR7
C	-5	PHE	-	expression tag	UNP Q9NXR7
C	-4	GLN	-	expression tag	UNP Q9NXR7
C	-3	GLY	-	expression tag	UNP Q9NXR7
C	-2	GLY	-	expression tag	UNP Q9NXR7
C	-1	GLY	-	expression tag	UNP Q9NXR7
C	0	ARG	-	expression tag	UNP Q9NXR7
H	-18	MET	-	initiating methionine	UNP Q9NXR7
H	-17	HIS	-	expression tag	UNP Q9NXR7
H	-16	HIS	-	expression tag	UNP Q9NXR7
H	-15	HIS	-	expression tag	UNP Q9NXR7
H	-14	HIS	-	expression tag	UNP Q9NXR7
H	-13	HIS	-	expression tag	UNP Q9NXR7
H	-12	HIS	-	expression tag	UNP Q9NXR7
H	-11	VAL	-	expression tag	UNP Q9NXR7
H	-10	ASP	-	expression tag	UNP Q9NXR7
H	-9	GLU	-	expression tag	UNP Q9NXR7
H	-8	ASN	-	expression tag	UNP Q9NXR7
H	-7	LEU	-	expression tag	UNP Q9NXR7
H	-6	TYR	-	expression tag	UNP Q9NXR7
H	-5	PHE	-	expression tag	UNP Q9NXR7
H	-4	GLN	-	expression tag	UNP Q9NXR7
H	-3	GLY	-	expression tag	UNP Q9NXR7
H	-2	GLY	-	expression tag	UNP Q9NXR7
H	-1	GLY	-	expression tag	UNP Q9NXR7
H	0	ARG	-	expression tag	UNP Q9NXR7

- Molecule 4 is a protein called BRISC and BRCA1-A complex member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	237	Total	C	H	N	O	S	0	0
			3761	1206	1872	306	359	18		
4	I	237	Total	C	H	N	O	S	0	0
			3761	1206	1872	306	359	18		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-22	MET	-	initiating methionine	UNP Q9NWX8
D	-21	ALA	-	expression tag	UNP Q9NWX8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	SER	-	expression tag	UNP Q9NWX8
D	-19	TRP	-	expression tag	UNP Q9NWX8
D	-18	SER	-	expression tag	UNP Q9NWX8
D	-17	HIS	-	expression tag	UNP Q9NWX8
D	-16	PRO	-	expression tag	UNP Q9NWX8
D	-15	GLN	-	expression tag	UNP Q9NWX8
D	-14	PHE	-	expression tag	UNP Q9NWX8
D	-13	GLU	-	expression tag	UNP Q9NWX8
D	-12	LYS	-	expression tag	UNP Q9NWX8
D	-11	VAL	-	expression tag	UNP Q9NWX8
D	-10	ASP	-	expression tag	UNP Q9NWX8
D	-9	GLU	-	expression tag	UNP Q9NWX8
D	-8	ASN	-	expression tag	UNP Q9NWX8
D	-7	LEU	-	expression tag	UNP Q9NWX8
D	-6	TYR	-	expression tag	UNP Q9NWX8
D	-5	PHE	-	expression tag	UNP Q9NWX8
D	-4	GLN	-	expression tag	UNP Q9NWX8
D	-3	GLY	-	expression tag	UNP Q9NWX8
D	-2	GLY	-	expression tag	UNP Q9NWX8
D	-1	GLY	-	expression tag	UNP Q9NWX8
D	0	ARG	-	expression tag	UNP Q9NWX8
I	-22	MET	-	initiating methionine	UNP Q9NWX8
I	-21	ALA	-	expression tag	UNP Q9NWX8
I	-20	SER	-	expression tag	UNP Q9NWX8
I	-19	TRP	-	expression tag	UNP Q9NWX8
I	-18	SER	-	expression tag	UNP Q9NWX8
I	-17	HIS	-	expression tag	UNP Q9NWX8
I	-16	PRO	-	expression tag	UNP Q9NWX8
I	-15	GLN	-	expression tag	UNP Q9NWX8
I	-14	PHE	-	expression tag	UNP Q9NWX8
I	-13	GLU	-	expression tag	UNP Q9NWX8
I	-12	LYS	-	expression tag	UNP Q9NWX8
I	-11	VAL	-	expression tag	UNP Q9NWX8
I	-10	ASP	-	expression tag	UNP Q9NWX8
I	-9	GLU	-	expression tag	UNP Q9NWX8
I	-8	ASN	-	expression tag	UNP Q9NWX8
I	-7	LEU	-	expression tag	UNP Q9NWX8
I	-6	TYR	-	expression tag	UNP Q9NWX8
I	-5	PHE	-	expression tag	UNP Q9NWX8
I	-4	GLN	-	expression tag	UNP Q9NWX8
I	-3	GLY	-	expression tag	UNP Q9NWX8
I	-2	GLY	-	expression tag	UNP Q9NWX8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP Q9NWX8
I	0	ARG	-	expression tag	UNP Q9NWX8

- Molecule 5 is a protein called Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	440	Total	C	H	N	O	S	0	0
			6893	2172	3452	616	638	15		
5	J	440	Total	C	H	N	O	S	0	0
			6893	2172	3452	616	638	15		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-23	MET	-	initiating methionine	UNP P34897
E	-22	GLY	-	expression tag	UNP P34897
E	-21	SER	-	expression tag	UNP P34897
E	-20	SER	-	expression tag	UNP P34897
E	-19	HIS	-	expression tag	UNP P34897
E	-18	HIS	-	expression tag	UNP P34897
E	-17	HIS	-	expression tag	UNP P34897
E	-16	HIS	-	expression tag	UNP P34897
E	-15	HIS	-	expression tag	UNP P34897
E	-14	HIS	-	expression tag	UNP P34897
E	-13	SER	-	expression tag	UNP P34897
E	-12	SER	-	expression tag	UNP P34897
E	-11	GLY	-	expression tag	UNP P34897
E	-10	LEU	-	expression tag	UNP P34897
E	-9	VAL	-	expression tag	UNP P34897
E	-8	PRO	-	expression tag	UNP P34897
E	-7	ARG	-	expression tag	UNP P34897
E	-6	GLY	-	expression tag	UNP P34897
E	-5	SER	-	expression tag	UNP P34897
E	264	THR	ALA	cloning artifact	UNP P34897
J	-23	MET	-	initiating methionine	UNP P34897
J	-22	GLY	-	expression tag	UNP P34897
J	-21	SER	-	expression tag	UNP P34897
J	-20	SER	-	expression tag	UNP P34897
J	-19	HIS	-	expression tag	UNP P34897
J	-18	HIS	-	expression tag	UNP P34897
J	-17	HIS	-	expression tag	UNP P34897
J	-16	HIS	-	expression tag	UNP P34897

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-15	HIS	-	expression tag	UNP P34897
J	-14	HIS	-	expression tag	UNP P34897
J	-13	SER	-	expression tag	UNP P34897
J	-12	SER	-	expression tag	UNP P34897
J	-11	GLY	-	expression tag	UNP P34897
J	-10	LEU	-	expression tag	UNP P34897
J	-9	VAL	-	expression tag	UNP P34897
J	-8	PRO	-	expression tag	UNP P34897
J	-7	ARG	-	expression tag	UNP P34897
J	-6	GLY	-	expression tag	UNP P34897
J	-5	SER	-	expression tag	UNP P34897
J	264	THR	ALA	cloning artifact	UNP P34897

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Zn	0
			1	1	
6	B	1	Total	Zn	0
			1	1	

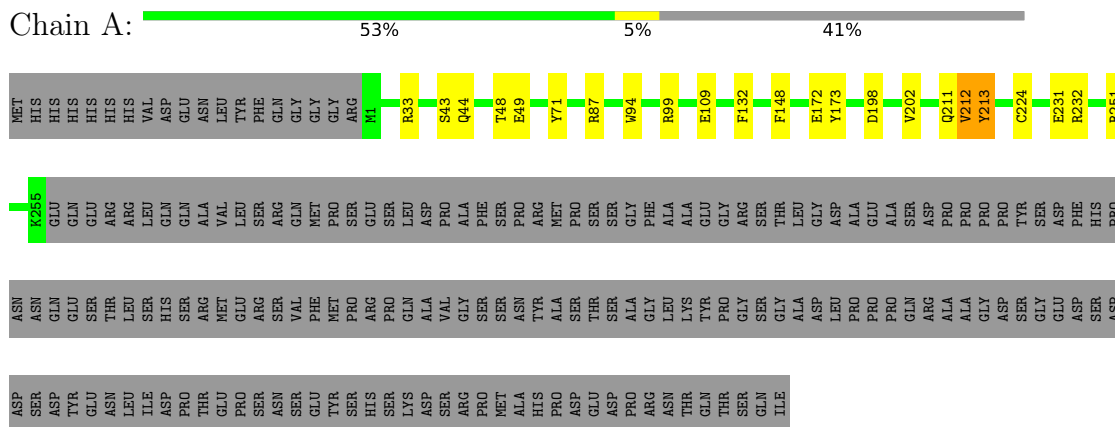
- Molecule 7 is water.

Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	H	O	0
			3	2	1	
7	G	1	Total	H	O	0
			3	2	1	

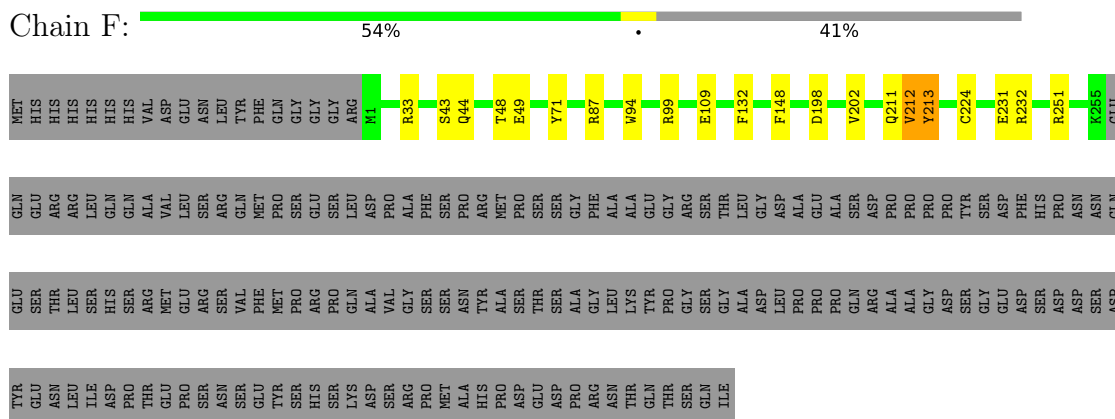
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

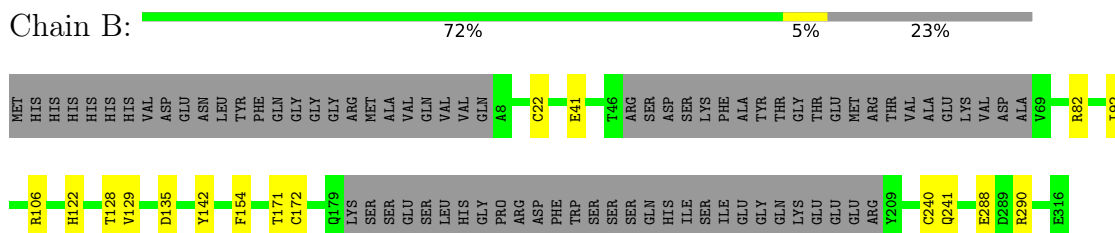
- Molecule 1: BRISC complex subunit Abraxas 2



- Molecule 1: BRISC complex subunit Abraxas 2

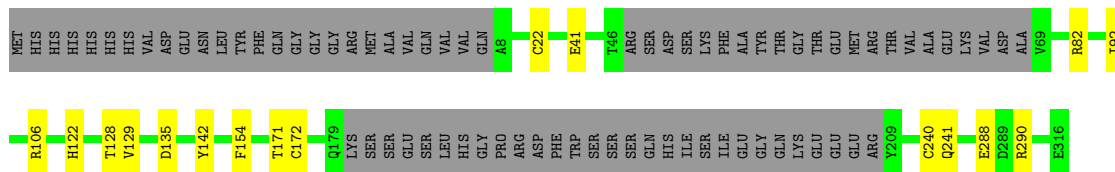


- Molecule 2: Lys-63-specific deubiquitinase BRCC36

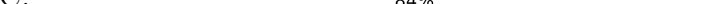


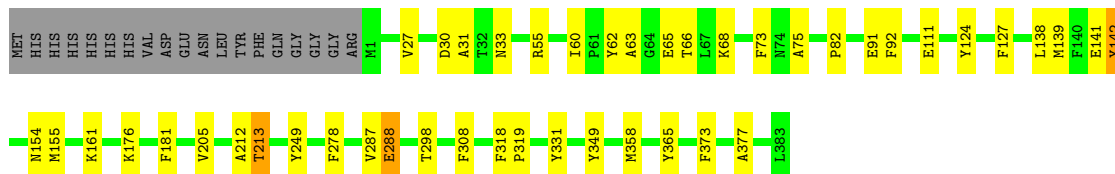
- Molecule 2: Lys-63-specific deubiquitinase BRCC36

Chain G: 72% 5% 23%

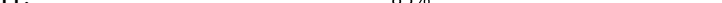


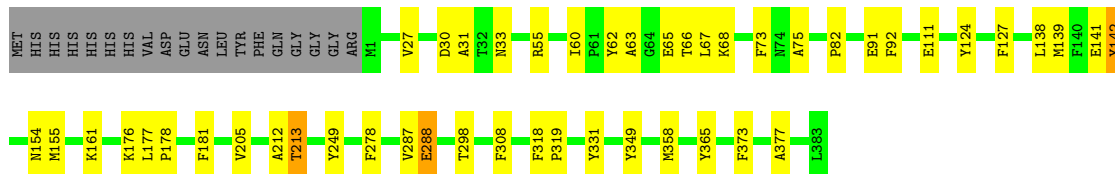
- Molecule 3: BRISC and BRCA1-A complex member 2

Chain C:  84% 10% • 5%



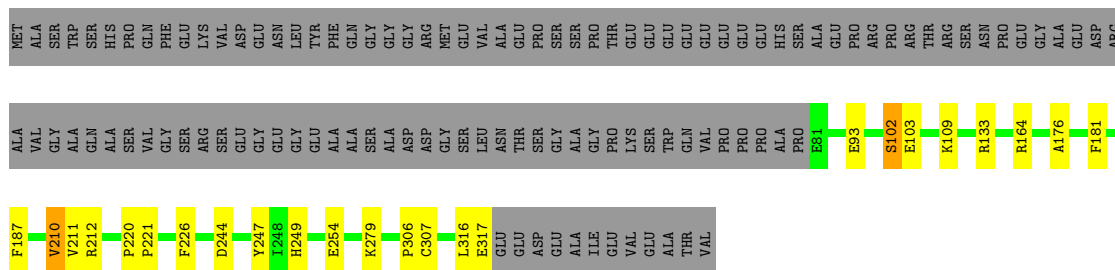
- Molecule 3: BRISC and BRCA1-A complex member 2

Chain H:  83% 11% 5%



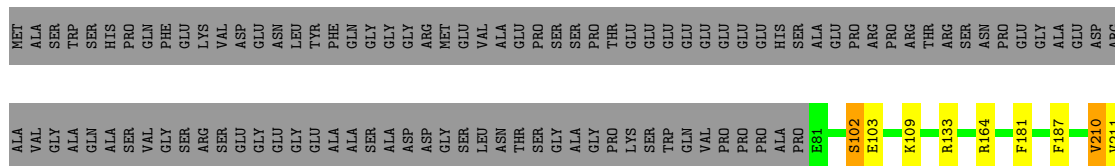
- Molecule 4: BRISC and BRCA1-A complex member 1

Chain D:  61% 6% • 33%



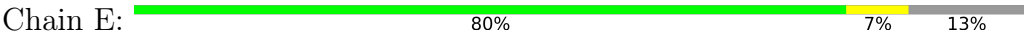
- Molecule 4: BRISC and BRCA1-A complex member 1

Chain I:  62% 5% 33%

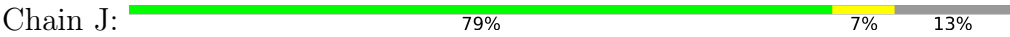




● Molecule 5: Serine hydroxymethyltransferase, mitochondrial



● Molecule 5: Serine hydroxymethyltransferase, mitochondrial



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	35595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF was determined using GCTF. CTF was corrected within RELION.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	58140	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.16	9/2120 (0.4%)	0.95	8/2856 (0.3%)
1	F	1.15	9/2120 (0.4%)	0.95	8/2856 (0.3%)
2	B	1.15	5/2105 (0.2%)	0.89	3/2845 (0.1%)
2	G	1.15	5/2105 (0.2%)	0.89	3/2845 (0.1%)
3	C	1.08	13/3169 (0.4%)	1.01	10/4310 (0.2%)
3	H	1.08	13/3169 (0.4%)	1.02	10/4310 (0.2%)
4	D	1.08	4/1934 (0.2%)	1.09	7/2623 (0.3%)
4	I	1.08	3/1934 (0.2%)	1.09	7/2623 (0.3%)
5	E	1.08	4/3508 (0.1%)	0.99	15/4744 (0.3%)
5	J	1.08	5/3508 (0.1%)	0.99	14/4744 (0.3%)
All	All	1.10	70/25672 (0.3%)	0.99	85/34756 (0.2%)

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	141	GLU	CD-OE2	-7.21	1.17	1.25
3	H	141	GLU	CD-OE2	-7.19	1.17	1.25
2	B	288	GLU	CG-CD	-7.16	1.41	1.51
1	A	224	CYS	CB-SG	-7.12	1.70	1.82
1	F	224	CYS	CB-SG	-7.10	1.70	1.82

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	212	ARG	NE-CZ-NH2	-11.28	114.66	120.30
4	I	212	ARG	NE-CZ-NH2	-11.27	114.67	120.30
5	J	288	TYR	CB-CG-CD2	-9.70	115.18	121.00
5	E	288	TYR	CB-CG-CD2	-9.68	115.19	121.00
3	C	142	TYR	CB-CG-CD2	-8.58	115.85	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2082	2052	2054	6	0
1	F	2082	2052	2054	5	0
2	B	2069	2053	2051	4	0
2	G	2069	2053	2051	4	0
3	C	3078	2999	3001	14	0
3	H	3078	2999	3001	16	0
4	D	1889	1872	1871	8	0
4	I	1889	1872	1871	5	0
5	E	3441	3452	3451	10	0
5	J	3441	3452	3451	13	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
7	B	1	2	0	0	0
7	G	1	2	0	0	0
All	All	25122	24860	24856	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 82 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:SER:O	1:F:44:GLN:C	2.43	0.56
5:J:359:HIS:ND1	5:J:359:HIS:N	2.53	0.55
4:D:210:VAL:HG12	4:D:211:VAL:H	1.73	0.54
1:A:43:SER:O	1:A:44:GLN:C	2.43	0.54
4:D:316:LEU:O	4:D:317:GLU:C	2.47	0.53

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/434 (58%)	238 (94%)	14 (6%)	1 (0%)	36	74
1	F	253/434 (58%)	237 (94%)	15 (6%)	1 (0%)	36	74
2	B	252/335 (75%)	248 (98%)	4 (2%)	0	100	100
2	G	252/335 (75%)	248 (98%)	4 (2%)	0	100	100
3	C	381/402 (95%)	352 (92%)	26 (7%)	3 (1%)	21	62
3	H	381/402 (95%)	353 (93%)	25 (7%)	3 (1%)	21	62
4	D	235/352 (67%)	212 (90%)	22 (9%)	1 (0%)	36	74
4	I	235/352 (67%)	212 (90%)	22 (9%)	1 (0%)	36	74
5	E	436/507 (86%)	417 (96%)	17 (4%)	2 (0%)	31	71
5	J	436/507 (86%)	417 (96%)	17 (4%)	2 (0%)	31	71
All	All	3114/4060 (77%)	2934 (94%)	166 (5%)	14 (0%)	40	74

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	75	ALA
3	C	213	THR
3	H	75	ALA
3	H	213	THR
4	D	210	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/386 (60%)	232 (100%)	0	100	100
1	F	232/386 (60%)	232 (100%)	0	100	100
2	B	235/302 (78%)	234 (100%)	1 (0%)	92	96
2	G	235/302 (78%)	234 (100%)	1 (0%)	92	96
3	C	337/353 (96%)	336 (100%)	1 (0%)	93	96
3	H	337/353 (96%)	336 (100%)	1 (0%)	93	96
4	D	219/309 (71%)	218 (100%)	1 (0%)	90	95
4	I	219/309 (71%)	218 (100%)	1 (0%)	90	95
5	E	364/416 (88%)	364 (100%)	0	100	100
5	J	364/416 (88%)	364 (100%)	0	100	100
All	All	2774/3532 (78%)	2768 (100%)	6 (0%)	94	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	279	LYS
4	I	279	LYS
2	G	82	ARG
3	C	55	ARG
3	H	55	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.